Analysis of Structural and Electronic Properties of $ZrOs_2$ Laves Phase Compound

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ABSTRACT

The structural and electronic properties of $ZrOs_2$ intermetallic compound is studied using full potential linearized augmented plane wave (FP-LAPW) method within generalized gradient approximation (GGA). $ZrOs_2$ is crystallizes in $MgZn_2$-type Laves phase structure. The total energy are calculated using Birch Murnaghan's equation of state to find the equilibrium lattice parameter (a_0), Bulk modulus (B) and pressure derivative of bulk modulus (B') and are in good agreement with experimental and available theoretical results. The electronic properties reveal that $ZrOs_2$ is metallic in nature. Fermi surface plots are also confirmed the metallic nature of $ZrOs_2$ compound.

Keywords- Intermetallic compounds; Electronic properties; Fermi surfaces

I. INTRODUCTION

Osmium (Os) is a refractory noble metal; it is hard but brittle. It is the densest natural element found in platinum ores. It has low vapor pressure and very high melting point. The search for a new superhard material is great scientific interest in both experimental and theoretical research. Recently OsB_2 has attracted much attention as an hard material [1]. The intermetallic compounds synthesized with platinum group of metals (e.g. Ru, Rh, Pd, Ir, Pt and Os) and transition metal (TM) elements are of extensive technological importance ranging from cutting and polishing tools to wear-resistant coating [2].

Vera *et al.* [3] have reported the Laves phase compounds of rare earth and of Halfnium as noble metal using x-ray diffraction technique. Mahdouk *et al.* [4] have done the enthalpy of formation for Hf-Os and Os-Ti systems and the X-ray powder diffraction and electron probe microanalysis are used to check structural state and stoichiometry of each phase. Structural and phase transformations in quenched and aged Zr-Os alloys have been studied by Taluts *et al.* [5] using experimental techniques. Brades *et al.* [6] have studied and reported the lattice parameters and related structural properties of several intermetallic compounds using X-ray analysis. Recently Liu *et al.* [7] have studied the structural, mechanical and electronic properties of OsTM and $TMOs_2$ (TM = Ti, Zr and Hf) intermetallics using first principles calculations. Xing *et al.* [8] have reported the structural stability and enthalpies of formation of refractory intermetallics TM and TM_3 (T = Ti, Zr, Hf; M = Ru, Rh, Pd, Os, Ir, Pt) using first principles calculation. In conclusion, the enthalpy of formation for some of these compounds are measured experimentally but the results on these compounds particularly structural and electronic properties of are very limited so our work will be useful for future investigation both experimentally and theoretically.In the present paper, the structural and electronic properties of $ZrOs_2$ in hexagonal phase are calculated using FP-LAPW method.

II. METHOD OF CALCULATION

For calculating the structural and electronic properties of $ZrOs_2$ intermetallic compound, we need to know the equilibrium geometry of the compound. Our calculation were performed using full potential linearized augmented plane wave (FP-LAPW) method as implemented in the WIEN2k code [9] within generalized gradient approximation (GGA) in the scheme of Perdew Burke and Ernzerhof (PBE) [10]. $ZrOs_2$ compound is crystallizes in $MgZn_2$-type structure with space group $P6_3/mmc$ (194) as shown in Fig. 1 (a). The transition metal Zr is located at (0.3333, 0.6667, 0.063) and Os1 and Os2 atoms are located at (0, 0, 0), (0.833, 0.666, 0.250). The energy eigen value convergence was achieved by expanding the basis function up to $R_{MT}*K_{max}= 7$, where R_{MT} is the smallest atomic sphere radius in the unit cell and K_{max} gives the magnitude of the largest **k** vector in the plane wave expansion. The valence wave functions inside the spheres are expanded up to $l_{max} = 10$ while the charge density is Fourier expanded up to $G_{max} = 12$. The self consistent calculations are considered to converge when the total energy of the system is stable within 10^{-4} Ry. Energy to separate core and valence state is -6.0 Ry. Integrations in the Brillouin zone were performed using **k**-points generated with 4×4×2 mesh points.

III. RESULTS AND DISCUSSION

In order to obtain the ground state structural properties, we have carried out the total energy calculation of $ZrOs_2$ intermetallic compound using the FP-LAPW method. The minimization curve is shown in Fig 1(b). Using this minimization curve, the equilibrium lattice parameters (a_0), bulk modulus (B) and its pressure derivative (B') have been calculated by fitting to the Birch Murnaghan's equation of state [11]. The results are summarized in Table. 1 along with other experimental and available theoretical results. One can see from Table.1 that the calculated lattice constant a_0 and c_0 of $ZrOs_2$ are close to the experimental data and also agree well with the previous reported theoretical data [6,7] which indicate the reliability of the calculation.

The electronic properties of $ZrOs_2$ compound along the high symmetry directions Γ→Σ→M→K→Λ→Γ→Δ→A in the Brillouin zone are shown in Fig. 2 (b). To understand the clear elemental contribution and bonding mechanism, we have also plotted the total and projected density of states (TDOS and PDOS) and illustrated in Fig. 2 (a).The lowest lying bands in $ZrOs_2$ (Fig.2 (b)) around -8.0 eV - -10.0 eV are mainly due to '6s' states of Os and the band around -6.0 eV to the E_F are mainly composed due to '5d' states of Os and '4d' states of Zr. The small contribution of 'p' states of Zr can also be noticed from DOS profile (Fig. 2 a).The hybridization between 'd' states of Zr and Os an also be seen in DOS. The density of states at Fermi level ($N(E_F)$) for $ZrOs_2$ is 4.35 states/eV.

The Fermi surfaces (FS) of $ZrOS_2$ compound is plotted for the bands which cross the E_F and shown in Figs. 3 (a-d). It is well established that electronic states crossing the Fermi level are primarily responsible for the Fermi surface (FS) structure and always considered as a key quantity to understand the electronic structure of any metallic material. In case of $ZrOs_2$, there are four bands cross the E_F. The first sheet is due to hole pocket at M point and second sheet for band is due to electron pocket along M→K point. The third and fourth sheet in $ZrOs_2$ are due to mainly hole pocket at Σ point and at Δ point. The last sheet is merge sheet of all the bands.

Table 1: Calculated ground state properties for $ZrOs_2$ intermetallic compound

Solids	Space group	a_0 (Å)	c_0(Å)	B(GPa)	B'	$N(E_F)$(states/eV)
$ZrOs_2$	P63/mmc	5.2269	8.6160	274.9	4.41	4.35
Exp.		5.18[a]	8.6128[a]			
Theo.		5.2249[b]	8.51[b]			

[a]Ref. [6], [b]Ref. [7]

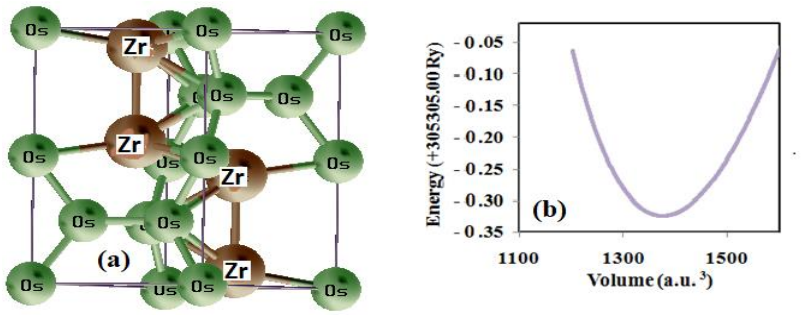

Figure 1: (a) Crystal structure (b) Energy vs Volume curve of AB_2 type C14 Laves phase compound

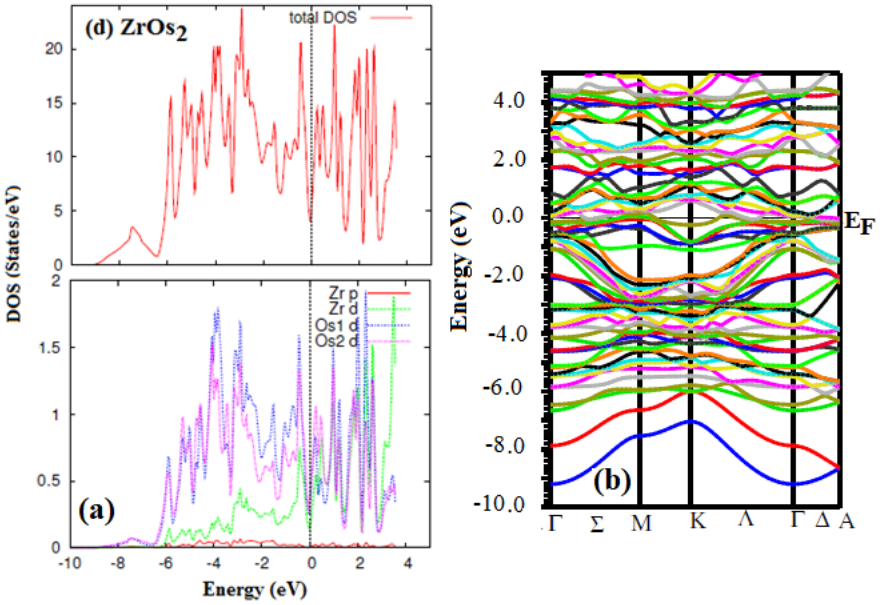

Figure 2: (a) Total and Partial density of states (b) Band structure of $ZrOs_2$

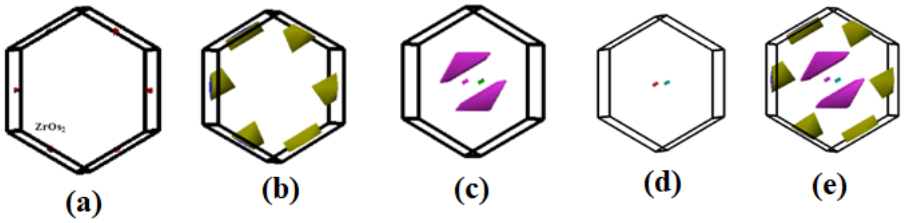

Figure 3: (a-d) Fermi Surfaces plots for $ZrOs_2$

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